OAK RIDGE National Laboratory

SCALE Covariance Approach

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WANDA February 28, 2022

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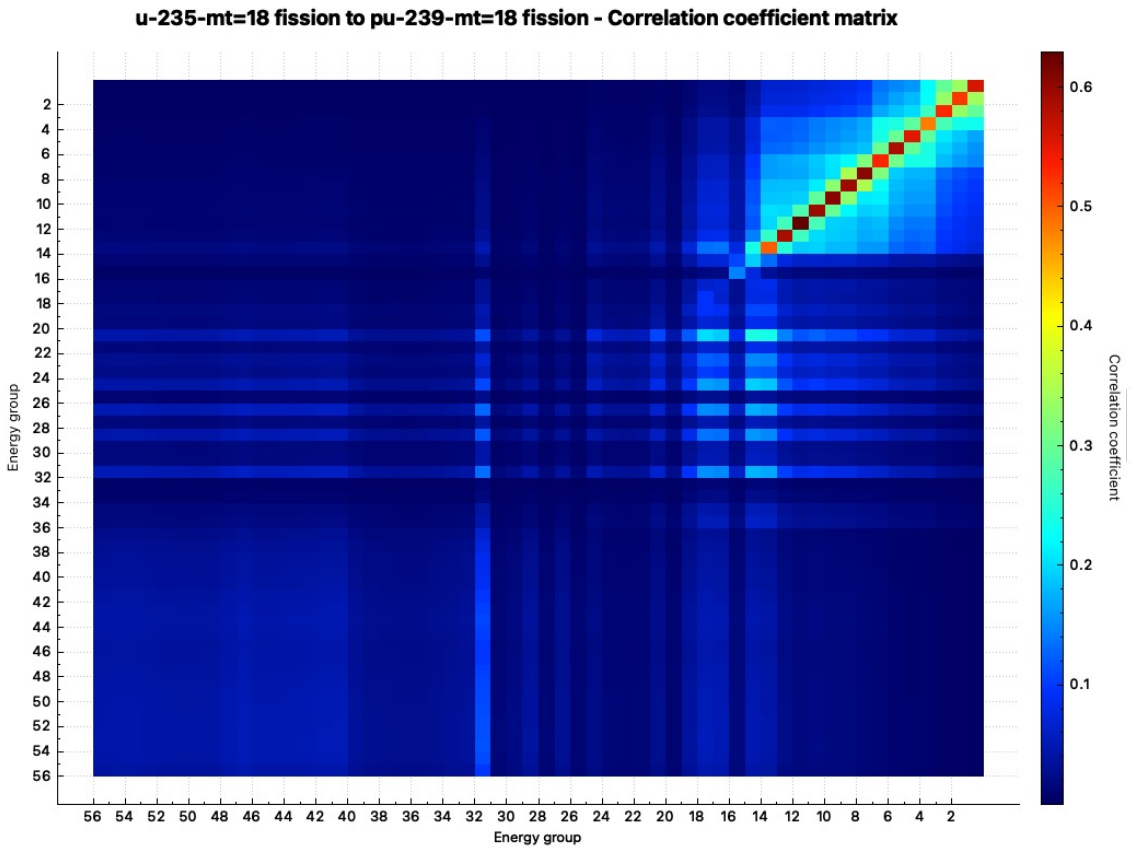
Brief history of covariance data in SCALE

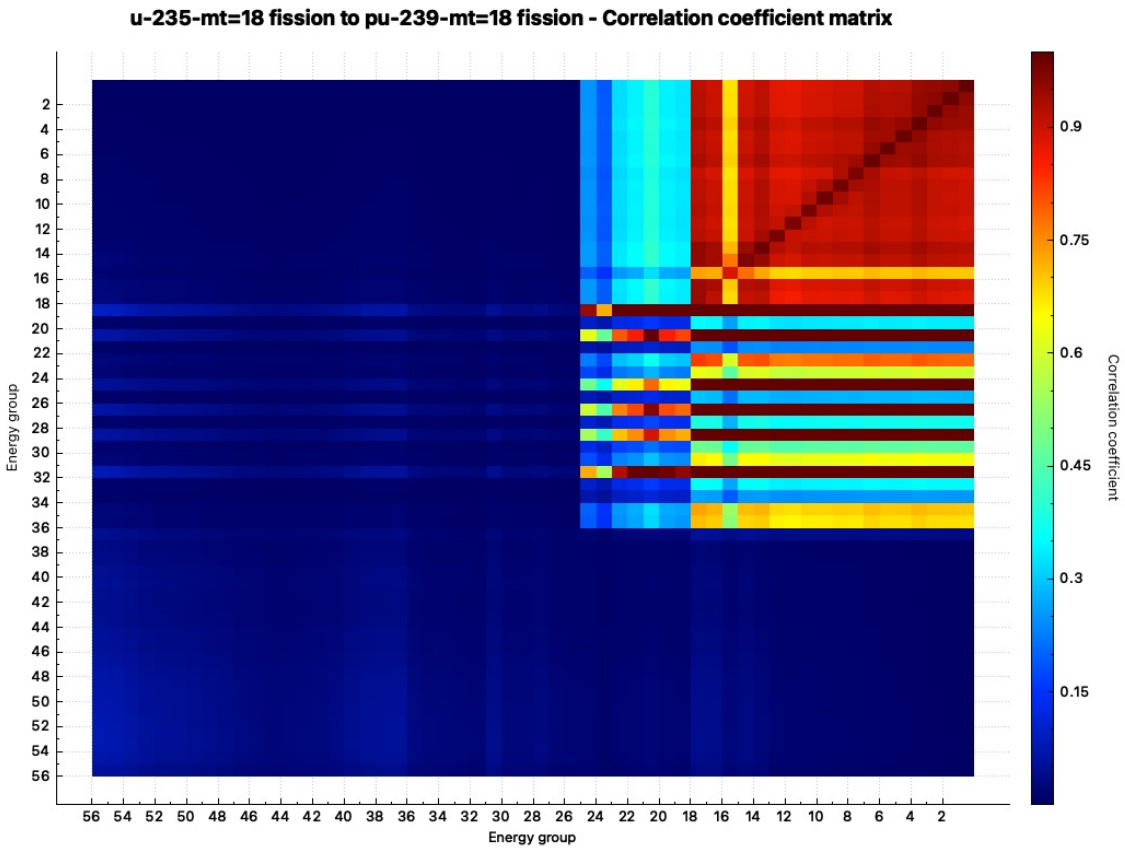
- SCALE-6
  - Creation of an applications-oriented covariance library
  - Franken-library
    - ENDF-7.0, ENDF-6, JENDL, BNL-LANL-ORNL (BLO) data
      - ORNL covariances based on the integral approximation below 5 keV
      - BNL/LANL above 5.0 keV
  - Importantly, gives SOME justifiable estimate for all materials (~277 mats)
- SCALE-6.3
  - ENDF-7.1
    - Covariance data for 190 isotopes
  - ENDF-8.0
    - Covariance data for 251 isotopes
  - Still patched with BLO data

Covariance Examples – Library changes

ENDF-7.1



ENDF-8.0



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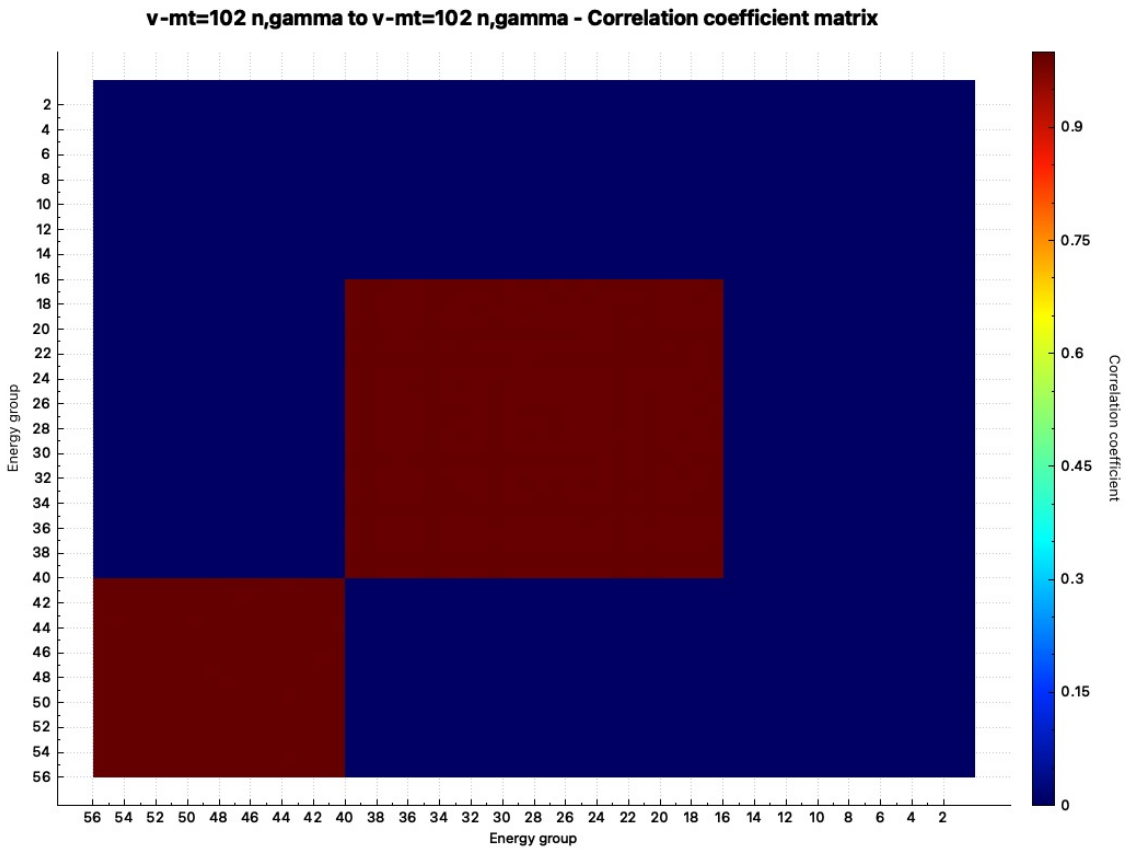
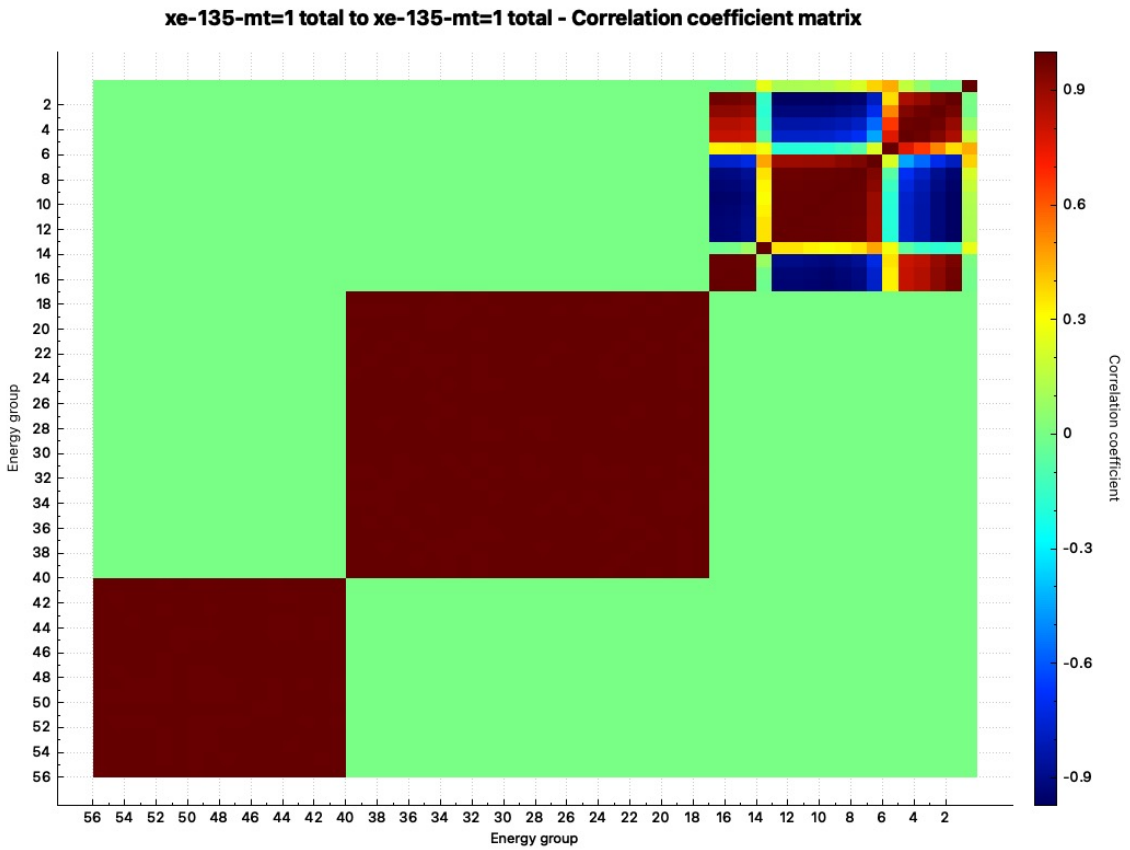
Covariance Examples Cont'd – Varying Fidelity

Vanadium Capture XS



Not in ENDF, estimated from Atlas of Neutron Resonances, same uncertainty and fully correlated in thermal and epithermal, no fast uncertainty

Xe-135 Total XS



Not in ENDF, estimated from Atlas of Neutron Resonances, same uncertainty and fully correlated in thermal and epithermal, fast uncertainty calculated purely by models, does not incorporate measurement uncertainty

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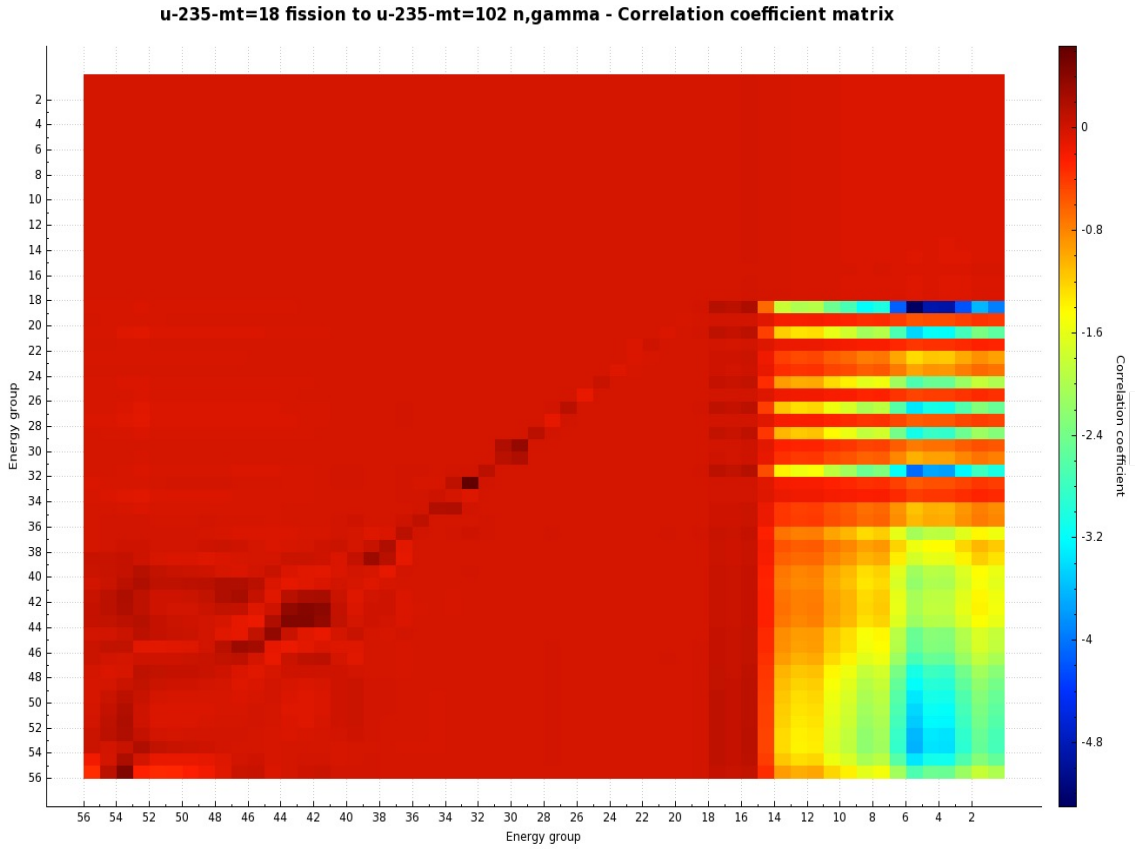
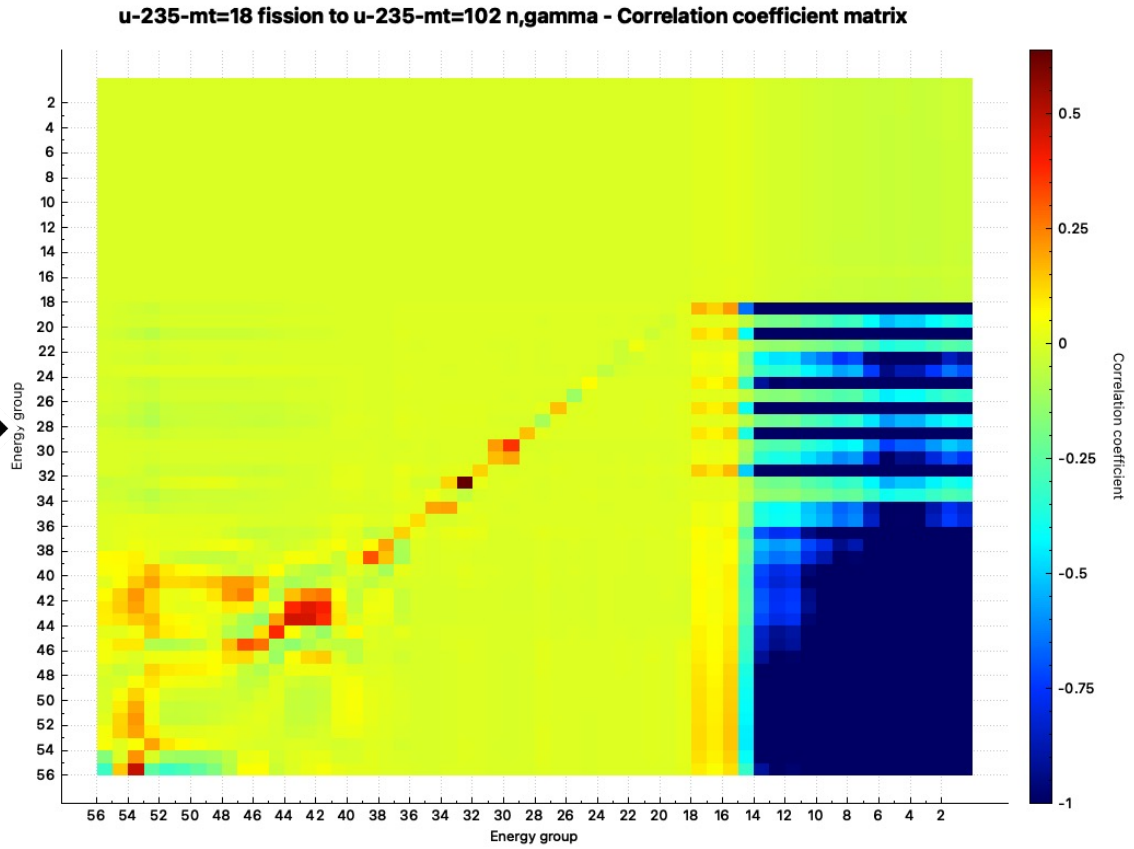
Covariance Examples Cont'd – Covariance Fixups

U-235 fission XS to U-235 capture XS





ENDF-8 problem in file, processing leads to correlation coefficients outside of [-1,1]

ENDF-8 patched, preserves intended covariance Information, correlation coefficients within valid range of [-1,1]

How do you fix mathematically incorrect covariances?

- If it is a minor roundoff problem, we bump the values back into the valid range, and report it (as in SCALE 6.2)
- If an egregious error (outside of precision) is detected for **ANY** matrix element, PUFF and COGNAC (AMPX covariance modules) will now:
  - Set self correlation matrices to the identity matrix
  - Set cross correlation matrices to the zero matrix
- In practice, this has only affected a small subset of isotopes in the ENDF-8 covariance library
- But how do you get the covariances to be consistent with the mean values?

Covariance fixup

- We don't know what integral experiments each evaluator used in tuning
  - Based on k-eff performance of ENDF-8 library with ICSBEP benchmarks, it certainly includes at least some subset of those benchmarks
- Here's what we did:
  - Fed ENDF-7.1/8 nominal 56-group covariance library and VALID inputs into TSURFER to compute an updated covariance matrix
  - Extracted the **new** correlations from adjusted covariance matrix calculated by TSURFER (leave all previously existing data intact)
  - Collapsed the new correlations to a three-group energy structure, roughly corresponding to the ICSBEP definition of thermal/intermediate/fast spectra
  - Expanded back to 56 groups, and add back to original ENDF-8 covariance library

References

1. W. A. Wieselquist, R. A. Lefebvre, and M. A. Jessee, Eds., ***SCALE Code System***, ORNL/TM-2005/39, Version 6.2.4, Oak Ridge National Laboratory, Oak Ridge, TN (2020).
2. D. Wiarda, M. E. Dunn, N. M. Green, M. L. Williams, C. Celik, L. M. Petrie, *AMPX-6: A Modular Code System for Processing ENDF/B*, ORNL/TM-2016/43 (2016).
3. V. Sobes, A. Holcomb, B.J. Marshall, T. Greene, D. Wiarda, W. A. Wieselquist, *Augmented ENDF/B-VIII.0 Covariance Library for SCALE 6.3*, Annals of Nuclear Energy, Volume 160 (2021).